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DIFFUSION IN BINARY PLASMA MIXTURES

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DIFFUSION IN BINARY PLASMA MIXTURES*

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This report considers ion diffusion in binary plasma mixtures. After first defining the diffusion coefficient for a binary mixture in Section I we show how it is related to concentration fluctuations in Section II. The relation between diffusion and self diffusion is discussed in Section III. Specializing to a model of classical ions in a uniform, charge neutralizing, background we discuss molecular dynamics simulations (Section IV) and kinetic theory calculations (Section V). Results for H^+-He^{++} mixtures at a temperature of 5 eV and $Si^{+14}-Sr^{+36}$ mixtures at 1 keV, all at 10^{22} ions/cm³, are presented and discussed in Section VI.

I. Defining Relations

We define the diffusion constant (also called the interdiffusion constant) as linearly relating mass fluxes to mass concentration gradients. Specifically for a type i particle let

$$\vec{j}_i(rt) = m_i n_i(r,t)(\vec{v}_i(r,t) - \vec{v}(r,t)) \quad (1.1)$$

where $n_i(r,t)$ is the number density for type i particles, $\vec{v}_i(r,t)$ its velocity field and $\vec{v}(r,t)$ the center of mass velocity defined by

$$\vec{v}(r,t) = \frac{\sum_{i=1}^2 m_i n_i(r,t) \vec{v}_i(r,t)}{\sum_{i=1}^2 m_i n_i(r,t)}. \quad (1.2)$$

This last relation implies that $j_1(rt) + j_2(rt) = 0$. Introducing mass densities, $\rho_i(r,t) = m_i n_i(r,t)$, and mass concentrations, $X_i(r,t) = \rho_i(r,t)/\rho(r,t)$, where $\rho(r,t) = \sum_i \rho_i(r,t)$ the diffusion constant, D , is formally defined by

$$j_i(r,t) = -\rho D \nabla X_i(r,t) \quad i = 1,2 \quad (1.3)$$

(In this equation and in what follows we often denote average quantities, such as ρ , by suppressing the space and time dependence.) Had we started with a two-by-two matrix of diffusion constants the relations $j_1(rt) = -j_2(rt)$ and $\nabla X_1(r,t) = -\nabla X_2(r,t)$ immediately reduce things back to Eq. (1.3). There is only one diffusion constant in a binary mixture. The self diffusion constant, which we define in Section III, is a microscopic concept and does not appear in a hydrodynamic or macroscopic description.

II. Green-Kubo Relation For The Diffusion Constant

The diffusion constant, like other transport constants, can be expressed in terms of fluctuations in the system in equilibrium; without any external forces to drive a particular mass or energy flux. Derivations of this are available in the literature [1,2] but for completeness we include a simplified derivation which gives the correct result. We consider low frequency, long wavelength fluctuations which is the regime governed by linear hydrodynamics. Since we are only interested in diffusion, we consider only mass concentration fluctuations and can ignore temperature and pressure fluctuations. Thus only number, and not momentum or energy conservation, must be considered. (For the full treatment see the references.)

The conservation law for, say, species one

$$\frac{\partial \rho_1}{\partial t}(rt) + \nabla \cdot \rho_1(rt) \vec{v}_1(rt) = 0 \quad (2.1)$$

may be rewritten using the definitions of Section I and overall number conservation as

$$\rho(r,t) \left(\frac{\partial X_1(r,t)}{\partial t} + \vec{v}(rt) \cdot \nabla X_1(r,t) \right) = -\nabla \cdot \vec{J}_1(rt) \quad (2.2)$$

Linearizing this equation and introducing the diffusion constant gives the diffusion equation for mass fluctuations

$$\frac{\partial}{\partial t} \delta X_1(r,t) = D \nabla^2 \delta X_1(r,t) \quad (2.3)$$

where $\delta X_1(r,t) = X_1(r,t) - \bar{X}_1$. The free space solution of this equation, in terms of Fourier components is

$$\delta X_1(k, t) = \delta X_1(k, 0) e^{-Dk^2 t} \quad (2.4)$$

If the initial fluctuation, $\delta X_1(k, t=0)$, is assumed to be an equilibrium fluctuation and we average over these initial fluctuations then

$$\langle \delta X_1(-k, t) \delta X_1(k, t=0) \rangle = \langle |\delta X_1(k, t=0)|^2 \rangle e^{-Dk^2 t} \quad (2.5)$$

or

$$\begin{aligned} \langle \delta X_1(-k, \omega) \delta X_1(k, t=0) \rangle &= \int_0^\infty e^{i\omega t} \langle \delta X_1(-k, t) \delta X_1(k, t=0) \rangle dt \\ &= \langle |\delta X_1(k, t=0)|^2 \rangle \frac{i\omega + Dk^2}{\omega^2 + D^2 k^4} \end{aligned} \quad (2.6)$$

where the bracket $\langle \rangle$ denotes an equilibrium ensemble average. Taking the appropriate limits in this last equation we obtain a relation for D

$$D \langle |\delta X_1(0, t) |^2 \rangle = \lim_{\omega \rightarrow 0} \lim_{k \rightarrow 0} \frac{\omega^2}{k^2} \operatorname{Re} \int_0^\infty e^{i\omega t} \langle \delta X_1(-k, t) \delta X_1(k, t=0) \rangle dt \quad (2.7)$$

Integrating by parts this becomes

$$D \langle |\delta X_1(0, t=0) |^2 \rangle = \lim_{\omega \rightarrow 0} \lim_{k \rightarrow 0} \frac{1}{k^2} \operatorname{Re} \int_0^\infty e^{i\omega t} \langle \dot{\delta X}_1(-k, t) \dot{\delta X}_1(k, 0) \rangle dt$$

To simplify this expression the mass fluctuation is rewritten in terms of mass densities as

$$X_1(rt) = \frac{\rho_1(rt)}{\rho(rt)} = X_1 + \frac{X_2 \delta \rho_1(rt) - X_1 \delta \rho_2(rt)}{\rho} + O(\delta \rho)^2 \quad (2.9)$$

Using the microscopic definitions for the mass densities, e.g.,

$$\rho_1(k, t) = \sum_{j \in 1} m_j e^{ik \cdot r_j(t)}$$

Eq. 2.8 becomes

$$D = \frac{1}{3\rho^2 \langle |\delta x_1(0, t=0)|^2 \rangle} \int_0^\infty \langle \vec{j}_D(t) \cdot \vec{j}_D(0) \rangle dt \quad (2.10)$$

$$\text{where } \vec{j}_D(t) = x_2 \sum_{i \in 1} m_1 \vec{v}_i(t) - x_1 \sum_{i \in 2} m_2 \vec{v}_i(t) \quad .$$

Using $\langle \vec{j}_D(0) \cdot \vec{j}_D(0) \rangle = 3kTMx_1x_2$, which follows from the Maxwell-Boltzmann velocity distribution, where M is the total mass of the system and introducing $S_{cc}(k)$, discussed below, by

$$\rho^2 \langle |\delta x_1(0, t=0)|^2 \rangle = \frac{m_1^2 m_2^2 N^3}{M^2} S_{cc}(k=0)$$

Eq. 2.10 reduces to

$$D = kt \left(\frac{C_1}{m_2} + \frac{C_2}{m_1} \right) \frac{C_1 C_2}{S_{cc}(k=0)} \int_0^\infty \frac{\langle \vec{j}_D(t) \cdot \vec{j}_D(0) \rangle}{\langle j_D^2 \rangle} dt \quad (2.11)$$

where the C 's are number concentrations. It is possible to factor the masses from this expression to obtain the form

$$D = \frac{1}{3C_1 C_2 N} \left[\frac{C_1 C_2}{S_{cc}(k=0)} \right] \int_0^\infty \langle \vec{v}_D(t) \cdot \vec{v}_D(0) \rangle dt \quad (2.12)$$

$$\text{with } \vec{v}_D(t) = C_2 \sum_{i \in 1} \vec{v}_i(t) - C_1 \sum_{i \in 2} \vec{v}_i(t) \quad .$$

The quantity $S_{cc}(k)$ is referred to as the concentration structure factor equivalently defined as the transform of

$$g_{cc}(r) = c_1^2 c_2^2 [g_{11}(r) + g_{22}(r) - 2 g_{12}(r)]$$

It also follows from thermodynamic arguments, starting from our definition in terms of fluctuations, that

$$S_{cc}(k=0) = NkT / \frac{\partial^2 G}{\partial c_1^2}$$

where G is the Gibbs free energy. In the small concentration limit ($c_1 \rightarrow 0$ or 1) $S_{cc}(k=0) \rightarrow c_1 c_2$. This is true at all concentrations in the case of an isotopic mixture, where classically only the ideal gas terms in the free energy depend on the concentration. In general, specifically for the model we treat below, this is not true but the usually small deviations can be evaluated theoretically or by simulation. The presence of the $c_1 c_2 / S_{cc}(k=0)$ factor stems from our definition of D in terms of the mass concentration gradient rather than the gradient of the chemical potential as is sometimes done.

Finally, it should be stressed that the various limits of long wavelength and low frequency fluctuations that have been invoked to obtain Eqs. (2.11) or (2.12) may be thought of as merely describing the particular experiments we use to obtain D . Once we have evaluated Eq. (2.12) either by simulation or kinetic theory the diffusion constant can be employed wherever the user dares.

III. Relation Between Diffusion and Self-Diffusion

Although it does not appear in the hydrodynamic description of a binary mixture, the process of self-diffusion is easily understood physically and refers to somehow marking (perhaps by isotopic substitution) one particle in

the mixture and observing how it drifts from its initial position. If this is repeated over numerous observations either with the same or a similar particle, the self-diffusion constant is defined from

$$\langle (\vec{r}_1(t) - \vec{r}_1(0))^2 \rangle \rightarrow 6D_1 t \quad (3.1)$$

for large t where the subscript 1 refers here to a type 1 particle. This can be rewritten in terms of the velocity autocorrelation function as

$$D_1 = \frac{1}{3} \int_0^{\infty} \langle \vec{v}_1(t) \cdot \vec{v}_1(0) \rangle dt \quad (3.2)$$

The current correlation for the diffusion constant is

$$\begin{aligned} \langle v_D(t) \cdot v_D(0) \rangle &= c_2^2 \sum_{i \in 1} \sum_{j \in 1} \langle \vec{v}_i(t) \cdot \vec{v}_j(0) \rangle \\ &\quad + c_1^2 \sum_{i \in 2} \sum_{j \in 2} \langle \vec{v}_i(t) \cdot \vec{v}_j(0) \rangle \\ &\quad - 2c_1 c_2 \sum_{i \in 1} \sum_{j \in 2} \langle \vec{v}_i(t) \cdot \vec{v}_j(0) \rangle \end{aligned}$$

Neglecting velocity correlations between different particles gives, using Eqs. (2.12) and (3.2), an approximate relation between the diffusion and self-diffusion constants,

$$\frac{S_{cc}}{c_1 c_2} D \approx c_2 D_1 + c_1 D_2 \quad (3.4)$$

This relation is exact in the low concentration limit. Further, if the diffusion current correlation of Eq. (3.3) is expanded in powers of t^2 it is seen that the cross correlations, which cause deviations from this relation, first enter at order t^4 .

In the simulations we concentrate on 50% mixtures where the deviations in this relation are likely to be largest. There is already some evidence in the literature on the reliability of the approximation, Eq. (3.4). In simulations on mixtures of rare gas liquids no deviation from this relation was observed to within the probably 5-10% accuracy of the simulations [3]. In a simulation of a model molten salt, where the anion and cation had equal mass and opposite charge so the diffusion and electric current are proportional, the relation 3.4 over-estimated the diffusion constant (and the conductivity) by about 20% due to the tendency of + and - pairs to diffuse together which produces no net current [4]. To get ahead of the story, in the present simulations we find that the approximation for D based on D_1 and D_2 gives an estimate within the uncertainty in our computed estimate for D for the $\text{Si}^{+14}\text{-Sr}^{+36}$ mixtures and slightly below the computed D for the $\text{H}^{+1}\text{-He}^{+2}$ mixture. Since self-diffusion constants are generally much easier to compute than diffusion constants this is a useful empirical rule.

IV. Some Remarks On The Simulations

The self and interdiffusion constants have been evaluated by molecular dynamics for a model of classical point ions in a uniform, charge neutralizing background. These techniques are by now routine, but questions were raised about the ensemble dependence of the computed time correlation function. The molecular dynamics simulations used a system at constant energy, particle number, volume, and total momentum. An ensemble of such systems is called a microcanonical ensemble. On the other hand the theoretical results have assumed a canonical or grand canonical ensemble. The differences between averages calculated in these ensembles and by molecular dynamics is due to the presence or absence of energy and momentum fluctuations. For example the

average square of the total momentum is zero in the molecular dynamics simulations but equal to $3 kTm$ for a canonical ensemble. Similarly the energy fluctuations, which are zero in a molecular dynamics simulation, are proportional to the specific heat in a canonical ensemble.

We are interested in the ensemble dependence of $\langle J_D(t) \cdot J_D(0) \rangle$. The key point is that the average diffusion current, J_D , is zero in the molecular dynamics experiment. This is still true even if the total momentum were non-zero since adding a drift velocity to all the velocities doesn't affect J_D . We also need a standard result in statistical mechanics that the ensemble dependence in the correlations of any two dynamical variables A and B is given by [5]

$$\begin{aligned} \langle \delta A \delta B \rangle_{ce} = & \langle \delta A \delta B \rangle_{MD} + \langle (E - \bar{E})^2 \rangle_{ce} \left(\frac{\partial \langle A \rangle_{MD}}{\partial E} \right) \left(\frac{\partial \langle B \rangle_{MD}}{\partial E} \right) \\ & + \langle P^2 \rangle_{ce} \left(\frac{\partial \langle A \rangle_{MD}}{\partial P} \right) \left(\frac{\partial \langle B \rangle_{MD}}{\partial P} \right) + 0 \left(\frac{1}{N} \right) \end{aligned} \quad (4.1)$$

where $\langle \rangle_{ce}$ denotes the canonical ensemble average. Applying this with $A = J_D(t)$, $B = J_D(0)$ we see that the ensemble dependent corrections vanish since $\langle J_D \rangle_{MD}$ is zero for all E and P. Therefore, the molecular dynamics correlation function can be used directly in the equations of Section II.

V. Kinetic Theory

The basic theoretical approach followed here is to express the time correlation function for the diffusion current in terms of the solution to a kinetic equation. The diffusion constant can then be expressed in terms of

the hydrodynamic matrix elements of the "memory" function appearing in the kinetic equation. More explicitly we write

$$D = \frac{1}{S_{CC}(k=0)} \operatorname{Re} \tilde{C}(0+i\eta)$$

where

$$\tilde{C}(z) = \int_0^{\infty} e^{izt} C(t) dt$$

and $C(t)$ is the diffusion current correlation function. Using the isotropy of the system one can write

$$\tilde{C}(z) = \sum_{\sigma=1}^2 \sum_{\tau=1}^2 \gamma_{\sigma} \gamma_{\tau} \int d^3 p d^3 p' \tilde{S}_{\sigma\tau}(k=0, z; pp') p_z p_z' \quad (5.1)$$

with

$$\gamma_1 \equiv \frac{c_2}{m_1/n}, \quad \gamma_2 \equiv \frac{-c_1}{m_2/n}.$$

The functions $\tilde{S}_{\sigma\tau}(k, z; pp')$ are the solutions to a kinetic equation of the form,

$$\begin{aligned} & \left(z - \frac{\vec{p} \cdot \vec{k}}{m_{\sigma}} \right) \tilde{S}_{\sigma\tau}(kz; pp') + \frac{\vec{p} \cdot \vec{k}}{m_{\sigma}} n_{\sigma} \phi_{\sigma}(p) \sum_{\sigma'} \tilde{C}_{\sigma\sigma'}(k) \int \tilde{S}_{\sigma'\tau}(kz; \vec{p}\vec{p}') d\vec{p} \\ & - \sum_{\sigma'} \int d\vec{p} \tilde{M}_{\sigma\sigma'}(kz; p\vec{p}) \tilde{S}_{\sigma'\tau}(kz; \vec{p}\vec{p}') \end{aligned} \quad (5.2)$$

$$= i n_{\sigma} \phi_{\sigma}(p) (\delta_{\sigma\tau} \delta(p-p') + n_{\tau} \phi_{\tau}(p') \tilde{h}_{\sigma\tau}(k)) .$$

In the above $\phi_{\sigma}(p)$ is the normalized Maxwell-Boltzmann distribution for

species σ , $\hat{h}_{\sigma\tau}(k)$ is the Fourier transform of $g_{\sigma\tau}(r) - 1$, $\hat{c}_{\sigma\tau}(k)$ the direct correlation function, and the $\hat{M}_{\sigma\tau}$'s are the "memory functions".

In order to solve this kinetic equation we will make two major approximations. The first concerns the explicit form of the memory function and the second concerns the method of solution. We use what is called the disconnected approximation for $\hat{M}_{\sigma\tau}$ [6] and our solution method is equivalent to a single sonine polynomial approximation [7].

Making these approximations we find [8]

$$D = \frac{c_1 c_2}{S_{cc}(k=0)} \left(\frac{\pi}{6}\right)^{1/2} \left(\frac{m_1 + m_2}{c_1 Z_1^2 m_2 + c_2 Z_2^2 m_1}\right)^{1/2} \frac{a^2 \omega_p}{Z_1^2 Z_2^2 \Gamma_0^{5/2} \Lambda} \quad (5.3)$$

where

$$\frac{4\pi}{3} a^3 = \frac{1}{n}, \quad \omega_p^2 = 4\pi e^2 \left(\frac{Z_1^2 n_1}{m_1} + \frac{Z_2^2 n_2}{m_2}\right),$$

$\Gamma_0 = e^2 / akT$ and Λ is a generalization of the Coulomb logarithm given by

$$\Lambda = \frac{-kT}{4\pi Z_1 Z_2 e^2} \left(\frac{kT(m_1 + m_2)}{2\pi m_1 m_2}\right)^{1/2} \frac{1}{2\pi n_1 n_2} \int_0^\infty dk k^2 \hat{c}_{12}(k) \int_{-\infty}^\infty d\omega [S_{11}(k\omega) S_{22}(k\omega) - S_{12}^2(k, \omega)] \quad (5.4)$$

To complete the calculation, we need an estimate of the dynamic structure factors in Eq. (5.4). These are approximated from the solutions to Eq. (5.2) with $\hat{M}_{\sigma\tau} = 0$.

A very similar method can be employed to obtain the self diffusion constants in a binary ionic mixture. These are presented along with the diffusion constants in Table I.

VI. Summary Of Results

Simulations and kinetic theory calculations have been carried out for a 50% H^+-He^{++} mixture at a temperature of ~ 5 eV and for several $Sr^{+36}-Si^{+14}$ mixtures at $T = 1$ keV. Results for diffusion and self-diffusion constants are given in Table I. The uncertainties in the molecular dynamics self diffusion constants, about 1%, are considerable less than the uncertainties in the diffusion constants, about 10%, since all particles of the same species may be averaged over. Several things are noteworthy in the table. First, as remarked earlier, the estimate of the diffusion constant based on the self diffusion constants is within the statistical uncertainty for the 50% Si-Sr mixture. Both the kinetic theory calculations and the simulations show little variation in D as the concentration is changed. The self diffusion constants, however, do decrease as more Sr is added and the plasma becomes more strongly coupled. As this occurs the interdiffusion is increasingly dominated by the more mobile Si ion with the result that the interdiffusion constant shows much less variation than the self diffusion constants. This should be generally true for other plasma mixtures. Finally, we remark that the time scale in the Si-Sr mixtures for diffusional spreading of ~ 100 Å is roughly 2 picoseconds at these temperatures.

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Table I: Self and interdiffusion constants in binary plasma mixtures.

MD					KT					
% Si	$D_{\text{Sr}^{+36}}$	$D_{\text{Si}^{+14}}$	$\frac{S_{cc}}{C_1 C_2} D$	$C_{\text{Sr}} D_{\text{Si}} + C_{\text{Si}} D_{\text{Sr}}$	$D_{\text{Sr}^{+36}}$	$D_{\text{Si}^{+14}}$	$\frac{S_{cc}}{C_1 C_2} D$	$C_{\text{Sr}} D_{\text{Si}} + C_{\text{Si}} D_{\text{Sr}}$	$\frac{S_{cc}}{C_1 C_2}$	Z^2 / Z^2
0.1						.185	.185	.185		
25.0	.088	.259	.215(17)	.217	.0775	.215	.186	.181	.923	.911
50.0	.105(1)	.325(3)	.217(10)	.215	.0904	.263	.182	.177	.860	.838
75.0	.128(2)	.408(4)	.204(15)	.197	.113	.349	.177	.172	.841	.807
99.9					.168		.168	.168		
% H ⁺	$D_{\text{He}^{++}}$	D_{H^+}	$\frac{S_{cc}}{C_1 C_2} D$	$C_{\text{He}} D_{\text{H}} + C_{\text{H}} D_{\text{He}}$	$D_{\text{He}^{++}}$	D_{H^+}	$\frac{S_{cc}}{C_1 C_2} D$	$C_{\text{He}} D_{\text{H}} + C_{\text{H}} D_{\text{He}}$	$\frac{S_{cc}}{C_1 C_2}$	Z^2 / Z^2
50%	.0488	.122	.0946(5)	.0854	.0418	.109	.082	.075	.914	.900

The two halves of the table (separated by the double line) give the results of molecular dynamics simulations (MD) and kinetic theory calculations (KT). For all cases $n = 10^{22}$ ions/cm³. $T = 1$ keV for the Si^{+14} - Sr^{+36} mixtures and ~ 5 eV for the H^+ - He^{++} mixture. The first column is number concentration (C). The D's labeled with a species subscript are for self-diffusion. All diffusion constants are in cm²/sec. The numbers in parenthesis give the estimated uncertainties in the least significant figure. The last column is the Debye-Hückel theory estimate for $S_{cc}(k=0)/C_1 C_2$.